DISCLAIMER

Materials and Molecular Research Division

Newsletter

March 1979
Volume 3, No. 3

HAPPY 100th BIRTHDAY ALBERT!

BULLETIN

Word has just been received that MMRD associates JOHN M. PRAUSNITZ and IAIN FINNIE have been elected to the National Academy of Engineering. Full details next issue.

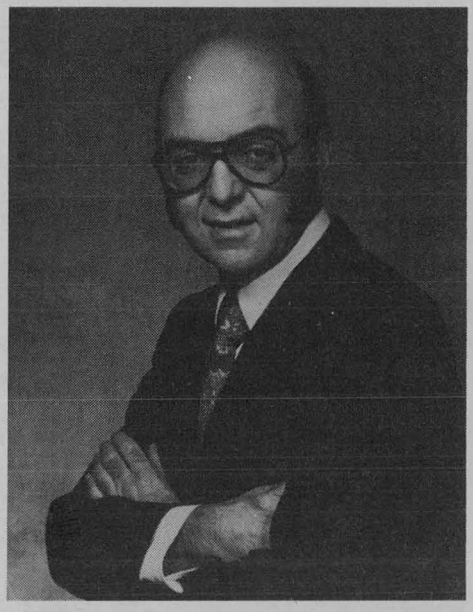
RESEARCH PROFILE

BROKEN-SYMMETRY STATES IN SOLIDS

L. M. Falicov

In is interesting to note that, under conditions of restricted energy availability, Nature usually chooses a state that is not very symmetric. The simplest example that comes to mind is a container with a gas inside. At high temperatures the gas, uniformly and isotropically, fills the container--a state of high symmetry indeed. As the temperature is lowered the gas liquifies and the liquid fills only a portion of the container. Although the uniformity of the space has been broken, each point in the space is still isotropic. At even lower temperatures, however, the liquid changes into a solid, with its characteristic crystal structure, and the isotropic properties of the liquid state are destroyed.

(Continued on page 4)



COHEN DOES IT AGAIN!

MARVIN L. COHEN, MMRD Investigator and UCB Professor of Physics, is the 1979 winner of the Oliver E. Buckley Solid State Physics Prize. This prize, endowed by Bell Laboratories, has been given since 1953 and its previous winners include such scientists as William Shockley, Charles Kittel, Walter Korn, T. H. Geballe, Erwin Hahn, and John Bardeen--illustrious company indeed!

DAVID SHIRLEY, Head of MMRD Division, describes him thusly: "MARVIN COHEN is the leading solid state theorist in the world today in applying computational methods to the surface electronic structure of real materials. The Oliver Buckley Prize is a fitting recognition of his contributions."

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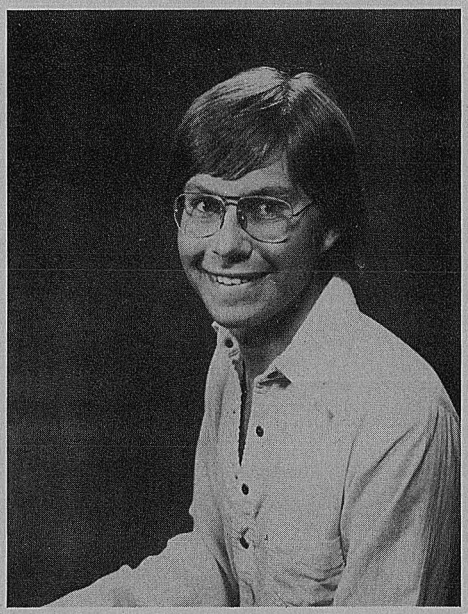

LAITONE WINS FIRST PRIZE

JONATHAN LAITONE won first prize for an article entered in a graduate division of the National Student Conference of the American Institute of Aeronautics and Astronautics (AIAA) for the 15th Annual Meeting in Washington, D.C. February 6-9. The winning paper was entitled, "Erosion Prediction Near a Stagnation Point Resulting from Aerodynamically Entrained Solid Particles."

LAITONE describes himself as a fluid dynamicist specializing in two-phase flow as applied to gasification of coal and the flow of char particles. What's that you ask, well--a fluid dynamicist is interested in the ways and reasons fluids move. Two-phase flow refers to the effects on each other and on the flow itself as well as on the carrier of two substances (in JONATHAN's case, his special interest is in reducing erosion effects). Gasification is the attempt to turn mined coal into methane gas used usually for heating purposes.

JONATHAN, a graduate student in the LEVY research group of MMRD, first entered his paper in the Western Division of the AIAA competition held at Pomona/Cal Poly. His success there led to an invitation to the nationals.

JON is still about a year away from his Ph.D., and was especially pleased to win the competition when he learned that many Ph.D. theses were among the entries!

JON received a certificate of award and a medallion during ceremonies at the awards dinner chaired by Senator Howard Cannon, Chairman of the Committee on Commerce, Science and Transportation.

Ironically, this award has normally carried a $1,000 grant but was presented this year without a stipend. However, AIAA did pay JON's way to Washington and home again.

LAITONE was born in Oakland, and attended school in El Cerrito and at Kennedy Hi in Richmond.

LAITONE has several active interests besides math and engineering. He is into photography--even had a show at the Berkeley Y-House following an earlier successful show in El Cerrito. He does comedy writing, occasionally preparing skits for presentation at local service clubs. He sings in the University Chorus, but rarely does John Denver impersonations!

Looking ahead, JON would like to teach mathematics which he feels many students shy away from because of its preparatory school presentation. He wants to try a historical approach with touches of humor and mystery to build student interest.

A few years ago, he designed a water system for his folk's cabin--and it worked. "It showed me," he says, "the real value of all this seemingly abstract course material!"

COHEN (continued)

This prize is awarded by the American Physical Society and is designed to recognize and encourage outstanding theoretical or experimental contributions to solid state physics. It consists of $5,000 and a certificate citing the contributions of the recipient. The Buckley is awarded for a most important contribution to the advancement of knowledge in solid state physics. The COHEN citation reads, "for timely explanations and novel predictions of electronic properties of solids through the imaginative use of quantum mechanical calculations."

Late last year while on his Guggenheim in Hawaii, COHEN was approached by a colleague who said, "I have good news and bad news for you." First, the bad news--you have to leave Hawaii and go to Chicago in March. Now the good news, you've won the Buckley Prize!"

COHEN also heard of the award in a second, interesting manner prior to his official notification. He happened to visit the office of the APS Executive Secretary, Bill Havens, and upon announcing himself to the secretary, got this response: "Oh, your name and a letter about you is taped to the file cabinet!" It was the official letter from the prize committee. COHEN quips, "I hear Havens has since been more concerned with office security and confidentiality."

Actual presentation occurred in Chicago at the Annual APS Meeting following a thirty-minute talk by him broadly covering the work for which he received the prize.

MARVIN's address was entitled, "The Pseudopotential Panacea." "I chose to talk about pseudopotentials because they have had a major influence on my research. I have centered much of my research on the behavior of electrons in solids. When electrons move through solids or whirl about the atomic nuclei in a solid, they interact with the nuclei and other electrons. These interactions can be very complicated. The pseudopotential is a device which allows the calculation of these complex interactions in a relatively simple way. I call the pseudopotential a panacea because this approach has yielded the solution of a large number of outstanding problems in solid state physics. Many properties are now predictable because of pseudopotentials."

And, we must add, because of MARVIN COHEN!

"Since there is a five-month period between first learning of the Oliver E. Buckley Prize decision and actual receiving of the award, it's possible to feel like a 'new' prizewinner for a long time.

I should add that the pseudopotential wasn't the only important component of my research program. The fine facilities at Berkeley were a very important resource. But the major ingredient was the superb group of graduate students and postdoctorals who have composed my group."

PASK & RISBUD WIN PURDY

Drs. JOSEPH A. PASK, MMRD Investigator, and SUBHASH H. RISBUD are the announced winners of the 1978 Ross Coffin Purdy Award "in recognition of their outstanding contributions to ceramic literature." The Award will be presented at the 81st Annual Meeting of the American Ceramic Society in Cincinnati, Ohio, April 28 - May 3, 1979.

SUBHASH received his Ph.D. at UCB in 1976 and is presently an Assistant Professor in the Materials Research Center at Lehigh University in Bethlehem, MD.

RESEARCH PROFILE (continued)

This continuous breaking of macroscopic symmetry as the temperature decreases is found throughout the realm of natural phenomena. Nowhere is it more evident and of more importance, however, than in the study of the properties of solids and, in particular, in the study of transitions between phases. These transitions occur under changes in external conditions, of which temperature, pressure, uniaxial stresses, electric and magnetic fields, and conditions of the surface are the most commonly controlled.

The most widely studied cases of broken symmetry states in solids have given rise to a new subfield of solid state physics: superconductivity, ferromagnetism, antiferromagnetism, ferroelectricity, and metal-insulator transitions. In each of these instances, as the temperature decreases, a given symmetry present in the high-temperature states is lost as the system undergoes a phase transition.

And in each case an observable quantity -- magnetization, electric dipole moment, energy gap in the optical spectrum -- can be considered to be a measure of the breaking of the symmetry. This observed quantity, usually called an order parameter, is such that it vanishes in the state of high symmetry. Experimental techniques are now developed to such an extent that the ways in which these order parameters change, how they compete against one another, and how they approach the zero value as the temperature increases and the macroscopic order is restored can be measured with extreme precision.

Most of the broken-symmetry-related phenomena are induced by the electronic properties of the solid, aided in most cases by the detailed interaction between electrons and the positive charge of the nuclei or ions which gives the solid its chemical signature. These electron and electron-ion mechanisms can produce symmetry-breaking in various ways, and there is an intense competition between states which, when subjected to very small changes in outside conditions, easily make transitions from one state to the other.

Two electrons, because of their identical charge, repel one another through a Coulomb force. However, the positive ions that make the solid, and which can be displaced from their equilibrium positions, constitute a polarizable medium. An electron, with its negative charge, polarizes the solid in a given region, and that polarization disturbance acts on other electrons as an attractive center. This results in an attractive electron-electron interaction mediated by the polarizable medium. The interaction is analogous to that of two steel balls placed on a rubber membrane; the balls tend to fall together into a common depression which they themselves produce in the elastic surface.

The repulsive Coulomb interaction and the attractive interaction mediated by the medium oppose one another and tend to break the symmetry in different ways. If the Coulomb repulsion dominates, magnetic phenomena or transitions between a metallic and an insulating state are to be expected. If the attractive interaction is the dominant one, the symmetry-breaking appears in the form of superconductivity or in the formation of ionic-type solids. In the latter phenomenon, known as a charge-density wave, the electronic charge is transferred from one site to another and tends to accumulate in given sites in a periodic fashion; our understanding of its properties and causes is relatively limited.

An illustration of the symmetry-breaking phenomenon is given in Fig. 1.

(Continued page 5)

RESEARCH PROFILE (continued)

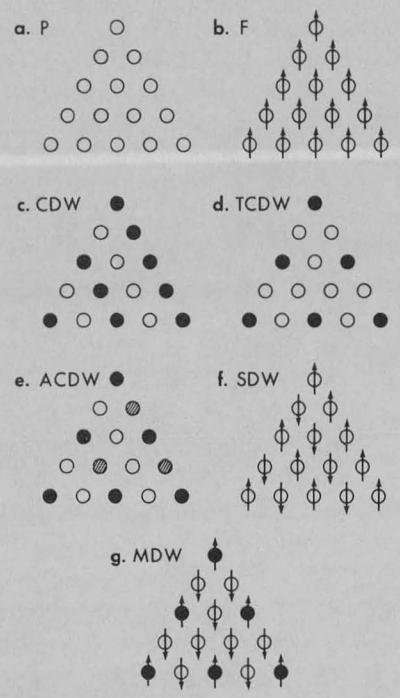

Fig. 1. Possible states in a hexagonal close packed layer. (a) The normal, symmetric paramagnetic state. (b) Ferromagnetic state. (c) A charge-density wave. (d) A triple charge-density wave. (e) An assymmetric charge-density wave. (f) An antiferromagnetic state also called spin-density wave. (g) A mixed-density wave including charge and spin periodic arrangements.

The first diagram shows a normal, paramagnetic (P) layer of atoms in a close-packed hexagonal layer; this is typical of a large number of substances in which broken-symmetry states are commonly found, for example, TaS_2 and $NbSe_2$. If the attractive interaction dominates, the symmetry of P breaks and states of nonuniform distribution of charge occur. Examples are (1) a charge-density wave (CDW), with stripes of alternating positive and negative charge; (2) a triple charge-density wave (TCDW), with a triangular distribution of charge; and (3) an asymmetric charge-density wave (ACDW) with alternating stripes, each stripe in turn showing nonuniform periodic distribution of charge.

If the dominant interaction is repulsive, each electron spin tends to repel the spin of opposite orientation, and magnetic states occur. We thus obtain a ferromagnetic state (F) if one spin prevails at all sites; however, other arrangements are also possible. Alternating rows of up and down spins constitute an antiferromagnetic state, also called a spin-density wave (SDW). It is even possible to obtain more complicated states (mixed density waves, MDW) in which neither the spin nor charge is uniform. Such a state is a ferrimagnet -- alternating spins but with an excess of one kind over the other -- as well as an ionic-like solid.

Broken-symmetry states produce fascinating experimental results related to their rich magnetic, electric, and crystal structures. In particular, diffraction experiments involving x-rays, neutrons, and electrons produce a variety and richness of texture that challenges the imagination. An example of electron microscopy diffraction patterns of multiple charge-density waves (MCDW) is shown in Fig. 2.

(Continued page 6)

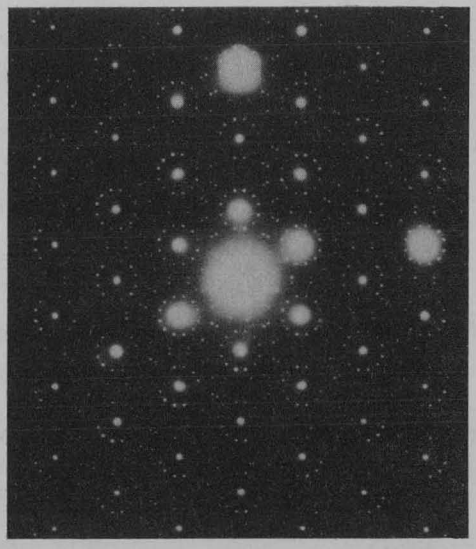

Fig. 2. An electron microscopy diffraction picture of a charge-density wave state in TaS_2 (Courtesy of Dr. J. Wilson, Bell Telephone Laboratories).

RESEARCH PROFILE (continued)

In addition to the most traditional cases of superconductivity, ferro-, ferri- and antiferromagnetism and ferroelectricity, known for decades if not centuries, new states of broken-symmetry are being explored and discovered. The discoveries are being made in such unrelated systems as organic solids, surface layers of semiconductors, and even in the electronic active layers of the devices (MOS FET) that constitute the ordinary chips of integrated circuits.

Another area of active research, both theoretical and experimental, is the study of competition between or coexistence of two different broken-symmetry states. For example, ferromagnetism and superconductivity are in close competition in some ternary compounds of rare earths and transition metals (e.g., $ErRh_4B_4$), superconductivity and antiferromagnetism in others, while charge-density waves and superconductivity tend to appear together in layered compounds and to coexist at some temperatures.

As any art lover can readily confirm, beauty can be defined as the broken symmetry of an empty canvas, an empty space, or an unbroken silence with a less symmetric but still comprehensible structure which our senses find harmonious.

GAS SAVING TIPS FREE

A free brochure listing 30 fuel-saving tips for drivers is available on request. Write to: Automotive Information Council, Box 273, Southfield, MI 48037.

One example from the brochure: For every five miles per hour over 50 there is a loss of one mile per gallon!

MMRD CONTRIBUTORS TO ART EXHIBIT

MMRD is well represented at the current Employees' Arts Council Mixed Media Show at the cafeteria. SANDRA STEWART is exhibiting five photographs, three from her recent trip to London (there's a stunning cat shot in this group!) and two pictures of skippers on flowers. DON KRIEGER has an acrylic, *Jazz at the Philharmonic*; a pastel chalk, *Backyard*; an oil, *Suspension*; and an oil chalk, *Blue*. ELAINE HEINEMANN is represented with two watercolors, *Bouquet #3* and *Spring Whimsey*. NANCY CHARPENTIER has photographs, *Road to Maui, Wyoming Table Top, Maroon Bells, Back Road to Berkeley, Wyoming Backdrop*, and *Hawaii Picnic*. ROY L. MCCOLLOUGH also has photographs in the show: *Big Sea, Big Sky; Forest Trail; Crowned African Cranes; Egmont, Canada;* and *Crater Lake Sentinel*.

The show at the LBL Cafeteria ends Friday, March 23.

LITERARY MAGAZINE

JULIE JONES, member of the EAC (Employees' Arts Council), and an organizer of a literary magazine for LBL employees, is looking for talent. Can you write short, short stories, articles, poems, satires, irony, or otherwise use basically lucid English?

JULIE is not only looking for material, but for editors and other assistants. If you have any ideals, or even ideas, please call JULIE at ext. 6715 (all calls should be at noon or after 5 p.m.) and make an offer while the bidding is still open.

All types of material, length, (excepting books!), and suitability to a general audience will be welcomed by JULIE.

PEOPLE NEWS

CHARLIE PEZZOTTI, Editor emeritus of this Newsletter, and his wife, MARY, have just returned from vacation to Louisiana (just in time to miss Mardi Gras), Florida and other points South. Maybe we can get him to come in and tell us all the amazing tales about the trip one lunchtime.

♦

MMRD had several students on the Chemistry volleyball team which recently completed a very successful season: FLOYD HOVIS, HENRY LUFTMAN, FRED GRIEMAN, MIKE BERMAN, PEGGY HOVIS, LINDA YOUNG and first alternate, STEVE HANSEN. They reached the IM Coed B League semi-finals, and achieved second place in a field of seventy teams.

♦

KATHY WILKINSON was recently in an auto accident in which her car was simply totalled! Fortunately, KATHY was apparently only bruised and is back at work.

♦

Professor JOSEPH A. PASK has been invited to present the annual Edward Orton, Jr. Memorial Lecture at the Annual Meeting of the American Ceramic Society to be held in Cincinnati, Ohio, this year.

Professor DENNIS W. HESS and his wife, Patricia, added a girl to their family on March 1, 1979.

SARAH ELIZABETH HESS was born at 5:40PM and joins another daughter, nine-year-old AMY. Congratulations!

♦

RON GRONSKY and KEN WESTMACOTT have officially moved into the new housing facility for the atomic resolution microscope. RON and KEN are located in Bldg. 72, Rm. 136, Ext. 5516.

SARA HARRIS has added a carved wooden redwood d r a g o n to her campus office. I can't quite decide whether he seems to be pouting or puffing--in any case SARA promises he won't bite visitors--but if sufficiently enraged, a rap on the head is possible.

♦

Dr. J. SINFELT, associated with EXXON Research Laboratories, visited several MMRD investigators March 7, 1979. Among those with whom he spoke were: ALEXIS BELL, LEO BREWER, DENNIS HESS, PETER VOLLHARDT, LEO FALICOV, HEINZ HEINEMANN, EARL MUETTERTIES, and DAVID CASTNER, sitting in for GABOR SOMORJAI.

♦

JENNI INGRAHAM, formerly a secretary with MMRD, is now attending Diablo Valley College taking preparatory courses to enter the field of metallurgy and engineering. Congratulations, JENNI.

♦

CARL LAMPERT recently attended the SERI/DOE Absorber Surfaces for Solar Receivers Conference in Boulder, CO. He reports that solar absorbers appear to be the most popular current area of investigation in solar thermal research.

In addition, CARL mentioned that the MMRD pure materials science approach to solar absorber coating was quite unique and excited much discussion--pro and con.

♦

HEINZ HEINEMANN was elected Councilor of the Fuels Division of the American Chemical Society to serve from March 1979 to March 1981. HEINZ will represent the Fuels Division at the regular ACS Council Meetings. Congratulations, HEINZ!

PEOPLE NEWS (continued)

HEINZ HEINEMANN attended the Oak Ridge National Labs Information Meeting of the Chemistry Division on March 19-21. He is a member of the Advisory Committee for that division.

♦

DAVE SHIRLEY slipped away from his magically paper-collecting desk recently to get in a weekend of scenic snowmobiling and skiing.

♦

GARETH THOMAS spent a hectic, but satisfying visit in the Republic of China attending the First Materials Symposium held there. The symposium was dedicated to him!

♦

GARETH worked his way home with lectures and presentations in Korea and Japan and arrived back to the good news that the Atomic Resolution Microscope project is moving right along.

♦

CAROL TUNG, formerly secretary for Professor MARVIN COHEN, has been promoted to the position of Undergraduate/Graduate Assistant II in the Physics Department at UCB. Congratulations, CAROL. Keep up the good work.

♦

SANDY STEWART traveled up to The Dallas, Oregon for the solar eclipse. It rained the day before, it rained the night before, and the morning of the eclipse dawned to fog. But SANDY drove on up to her selected lookout virtually daring the weather to interfere! And audacity paid off--it cleared completely just prior to the event. SANDY not only watched--she photographed it!

DEPARTMENT OF ENERGY
FY 1980 BUDGET

	Budget Authority		
	1978	1979	1980
	($ In Millions)		
Energy Technology	$3,373	$ 3,625	$3,583
Basic Sciences	406	431	474
Conservation	538	671	555
Regulation and Information	182	276	323
Defense Activities	2,562	2,685	3,022
Government-Owned Operations	738	248	149
Policy and Management	241	258	308
Less: Supplemental and Other Adjustments	-122	-403	—
Subtotal	$ 7,918	$ 7,791	$8,415
Strategic Petroleum Reserve	3,180	3,008	8
Total DOE Funding	$11,098	$10,799	$8,423

LBL REPORTS BY MMRD PERSONNEL

NOTE: All MMRD/LBL reports listed here are available in the reference section of the MMRD Library, Bldg. 62, Rm. 339, or call Marianne Larsen, Librarian, at Ext. 5971 (p.m. only)

LBL-7807: The Chemistry of Coal Model Compounds--Cleavage of Aliphatic Bridges Between Aromatic Nuclei Catalyzed By Lewis Acids... *N. D. Taylor* ... (M.S. thesis).

LBL-8205: The Oscillator Strength of the C_2 Swan Bands ... *L. Brewer and L. Hagan.*

LBL-8234: The He I Photoelectron Spectroscopy of Heavy Group IV-VI Diatomics ... *M. G. White, R. A. Rosenberg, S.-T. Lee and D. A. Shirley.*

LBL-8334: Syntheses and Electronic Structures of Decamethylmanganocenes ... *J. L. Robbins, N. M. Edelstein, S. R. Cooper and J. C. Smart.*

LBL-8335: Acoustic Emission Sources in Brittle Solids ... *A. G. Evans.*

LBL-8380: The CO-Precipitation of Vacancies and Carbon Atoms in Quenched Platinum ... *K. H. Westmacott and M. I. Perez.*

LBL-8441: Photochemical Processes at the Solid-Gas Interface: The Adsorption and Reactions of Gaseous CO_2 and H_2O on Pt-$SrTiO_3$ Single Crystal Sandwiches ... *J. C. Hemminger, R. Carr, W. J. Lo and G. A. Somorjai.*

LBL-8509: Mass Transfer Controlled Reactions in Packed Beds at Low Reynolds Numbers ... *P. S. Fedkiw* ... (Ph.D. thesis).

LBL-8521: Perturbation Solutions for the Particle Trajectories of a Gas-Solid Mixture Entering a Curved Duct ... *W.-S. Yeung.*

LBL-8544: Significance of Oxygen on Interstitial Ordering in Tantalum (The $Ta_{64}C$ Artifact) ... *U. Dahmen and G. Thomas.*

LBL-8592 Abs.: Free Exciton Lifetime and Diffusion in Ge ... *J. C. Culbertson and R. M. Westervelt.*

LBL-8599 Abs.: Dynamics of Photodissociation of O_3 ... *R. K. Sparks, L. R. Carlson, K. Shobatake, M. L. Kowalczyk and Y. T. Lee.*

LBL-8632: Microstructure and Optical Properties of Black Chrome Before and After Exposure to High Temperatures ... *C. M. Lampert and J. Washburn.*

LBL-8637: Experimental and Computational Study of HF + Xe Scattering ... *C. H. Becker, P. W. Tiedemann, J. J. Valentini, Y. T. Lee, and R. B. Walker.*

LBL-8642: Specific Sequestering Agents for the Actinides. 3. Polycatecholate Ligands Derived from 2,3-Dihydroxy-5-Sulfobenzoyl Conjugates of Diaza- and Tetraazaalkanes ... *F. L. Weitl and K. N. Raymond.*

LBL-8644: Hydroido[Tris (Hexamethyldisilylamido)]-Thorium(IV) and -Uranium(IV) ... *H. W. Turner, S. J. Simpson, and R. A. Andersen.*

LBL-8661: Microstructures and Phase Transformations in Interstitial Alloys of Tantalum ... *U. Dahmen* ... (Ph.D. thesis).

LBL-8666: Sixth Quarterly Report of Research on Cu_xS - (Cd,Zn)S Photovoltaic Solar Energy Converters ... *B. L. Chin, L. E. Sindelar and J. Washburn.*

LBL-8687: Imidazolium Tetrachlorodioxouranium(VI), $[C_3N_2H_5^+]_2$ $[UO_2Cl_4]^{-2}$ ... *D. L. Perry, D. P. Freyberg, and A. Zalkin.*

LBL-8741: Free Metal and Free Ligand Concentrations Determined From Titrations Using Only a pH Electrode. Partial Derivatives in Equilibrium Studies ... *A. Avdeef and K. N. Raymond.*

LBL-8766: Collisionless Non-Radiative Decay Rates of Single Rotational Levels of S_1 Formaldehyde ... *J. C. Weisshaar and C. B. Moore.*

LBL-8767: Resonant Multiphoton Dissociation and Mechanism of Excitation for Ethyl Chloride ... *H.-L. Dai, A. H. Kung, and C. B. Moore.*

CALENDAR

March 27: "The Relationship Between Science and Technology an Developing Countries," Michael Moravcsik, University of Oregon. Energy and Environment Division Seminar, Bldg. 90, Room 3143, 4:00 p.m.

SURFACE SCIENCE AND CATALYSIS SEMINARS, 1:00 p.m., Bldg. 62, Rm. 203

April 4: "Surface Studies of Catalysis by ESCA," Dr. R. T. Lewis, Chevron Research.

April 6: "CO Oxidation over Platinum," Dr. J. Wei, MIT.

April 11: "Catalyst-Support Interation, Some New Prospectives," Dr. M. Sheleff, Ford Motor Co.

April 18: "Olefin Disproportionation," Dr. R. Banks, Phillips Petroleum Co.

April 25: "Catalyst Poisoning," Prof. J. B. Butt, Northwestern Univ.

♦

August 20-22: "Fourth International Conference on Ellipsometry" LBL Contact: Dr. R. H. Muller.

♦

October 1979: International Energy Conservation Month.

MMRD NEWSLETTER ..... **March 1979**

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